Co-Optimization of
Fuels & Engines

Multi Mode: Fuel Property Impacts and limitations on combustion - SI focus

Derek Splitter (presenter)

Jim Szybist, Scott Sluder, Sibendu Som, Roberto Torelli, Hengjie Guo, Zongyu Yue (currently at Tianjin Univ. China)

Date 6/3/2020

Project ft069

2020 DOE Vehicle Technologies Office

Annual Merit Review

better fuels | better vehicles | sooner

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Overview

Timeline [a]

- Co-Optima 1.0: FY15-FY18
  → Complete
- Co-Optima 2.0: FY19-FY21
  → Approx. 58% complete

Budget

	FY19	FY20
E.1.1.2 Multicylinder SI Investigation to Support Multimode ACI/SI Strategies	$376K	$340K
F.1.16.1 Kinetic Modeling Support of ORNL Experiments	N/A	$130K
F.1.8.1 - Characterizing BOB Impacts and Limits within OI	$375K	$315K
F.1.5.2 Fuel Effects on Low Speed Pre-Ignition	$100K	$100K
G.1.10 Numerical Study on Auto-Ignition in Multimode Single-Cylinder Engine	$145K	$175K

a. FY19 is the start of the second 3-year funding period of the DOE lab-call projects. Note that the DOE FY starts on October 1 and ends on September 30.

Barriers

USCAR Priority 1: Dilute SI Combustion

- Knock Mitigation

→ *Developing a better understanding of how fuel properties can be predictive of knock*

USCAR Priority 3: Multimode ACI

- Increased tolerance to market fuel variability

→ *Developing a better understanding fuel autoignition under ACI conditions*

Partners

- Co-optima partners include nine national labs, one industry, 20+ universities, external advisory board, and stakeholders (80+ organizations)
- 15 Industry partners in the AEC MOU
- Task specific partners
- General Motors – Hardware
- Ford – Hardware
- Shell - Fuels
- LLNL (Pitz & Wagnon) – Chemical kinetics
- Convergent Science Inc. – Software
- Ansys - Software
- *+Many more – details in later slides*

Relevance

Overarching Co-Optima Relevance

- Internal combustion engines and liquid fuels will continue to dominate transportation for many years.
- Significant opportunities exist to further improve engine efficiency.
- Research into better integration of fuels and engines is critical to accelerating progress towards efficiency, environmental, and economic goals.

Presentation Specific Relevance

- Mitigation of knock is listed as a top priority research area in USDRIVE roadmap to attain higher efficiency for light-duty engines
- Increasing the tolerance to market fuel variation for ACI multimode combustion is also listed as a barrier in the USDRIVE roadmap
  - The work presented in this presentation informs our ability to predict knock for SI combustion and autoignition for ACI
  - Improved predictions are based on fuel properties, chemical kinetics, and CFD simulations

Milestones

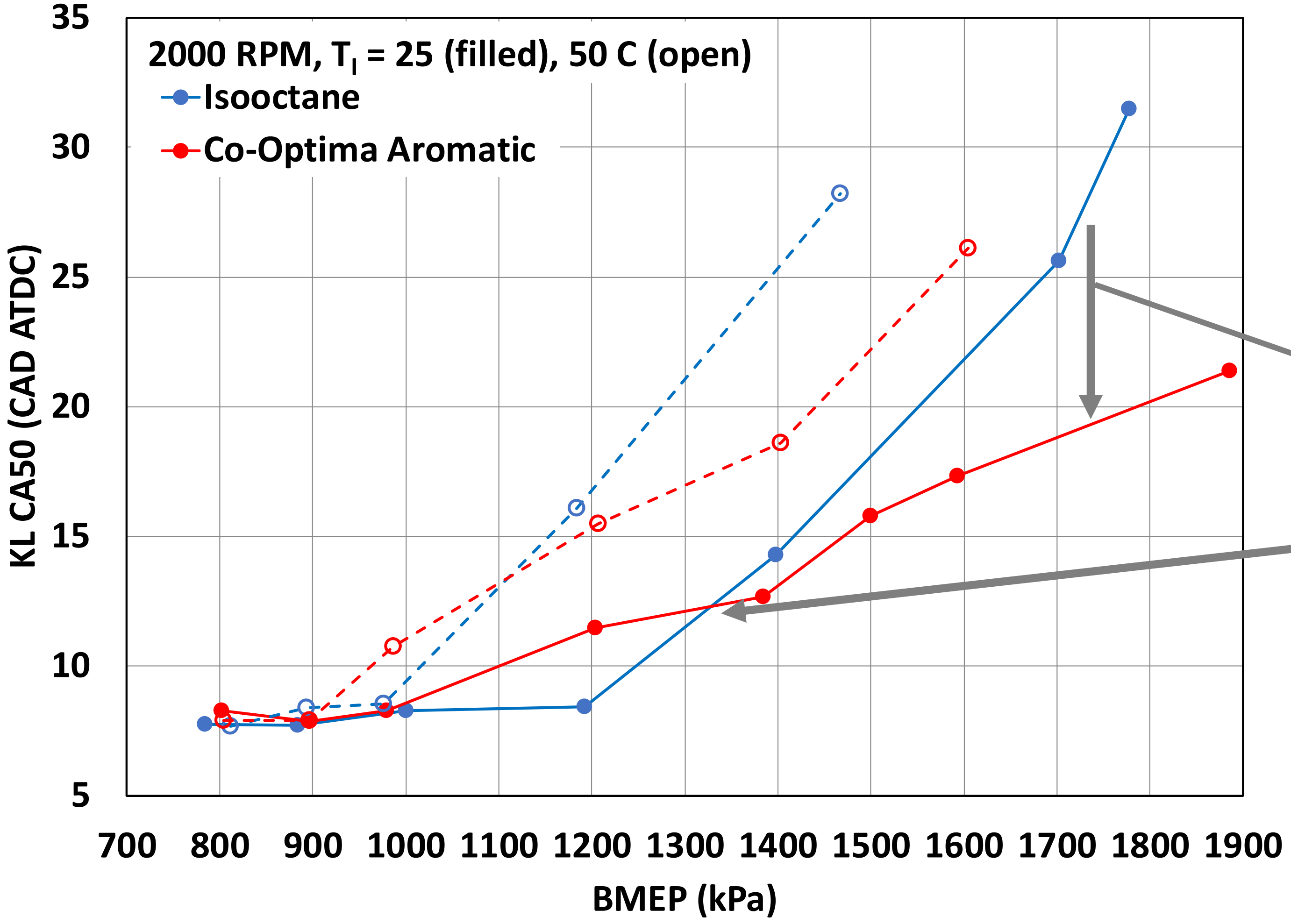
Month / Year	Project	Description of Milestone or Go/No-Go Decision	Status
06/2020	F.1.16.1	Complete modeling of 3 Co-Optima core fuels under MON-limited conditions, determine if models and experiments agree.	On-Track
9/2020	F.1.5.2	Complete LSPI testing with LIF diagnostic on 6 fuels or 3 fuels at 2 levels varying distillation and flame speed independently.	On-Track
9/2020	E.1.1.2	Determine MON requirements at increased compression ratios.	On-Track
06/2020	F.1.8.1	Supply data for consolidation task for the operable speed-load ACI range using the Co-Optima core fuels	On-Track

Approach Focuses on Experimental Study of the Importance of MON to Retain SI Power Density for Multimode ACI/SI Strategy

ORNL, Sluder: Approach

- Is there a power density trade-off in SI mode when octane sensitivity is maximized to enable ACI in multimode engines?
  - Focus on power density: stoichiometric high speed, high-load conditions needed for multimode implementations
- OS is explored with Co-Optima core fuels
- EcoBoost 1.6L Engine
  - OEM pistons: CR 10 (increase planned)
  - 79mm bore x 81.4mm stroke
  - Center-mount DI
  - Open ECU for control
- A closely linked kinetic modeling study to expand knowledge gained through experimentation is also underway
  - Task F.1.16.1

Initial Experiments Affirm That MON < RON is Beneficial at Low Engine Speeds and That it Remains so as Intake Temperature Increases



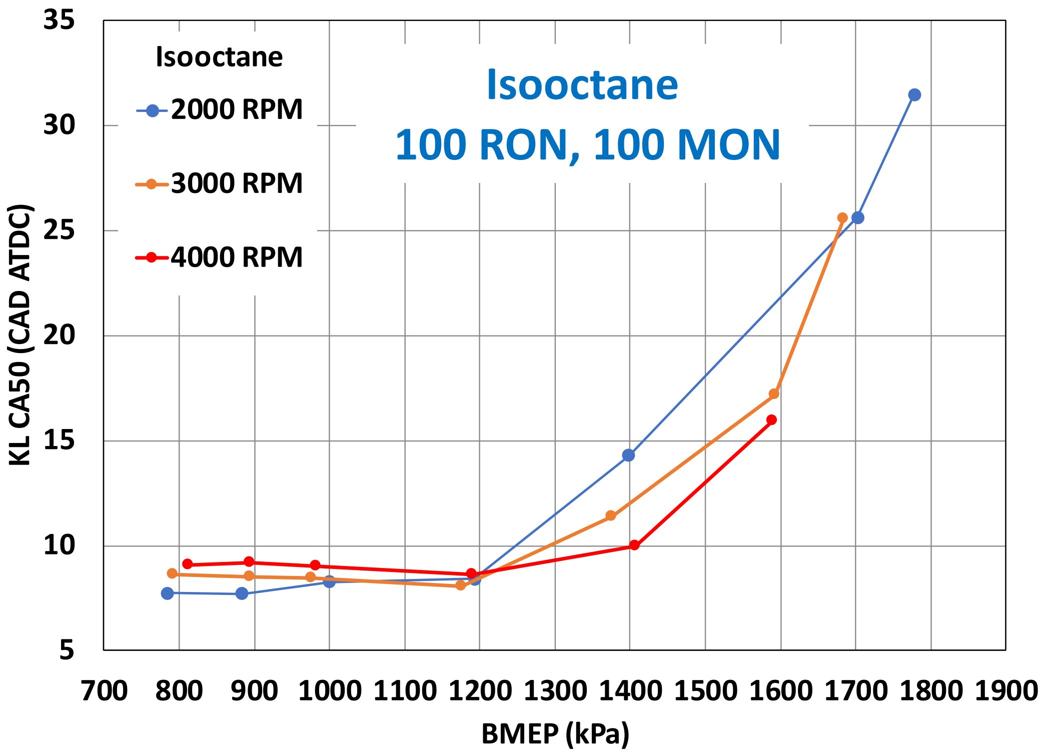
Isooctane: 100 RON, 100 MON

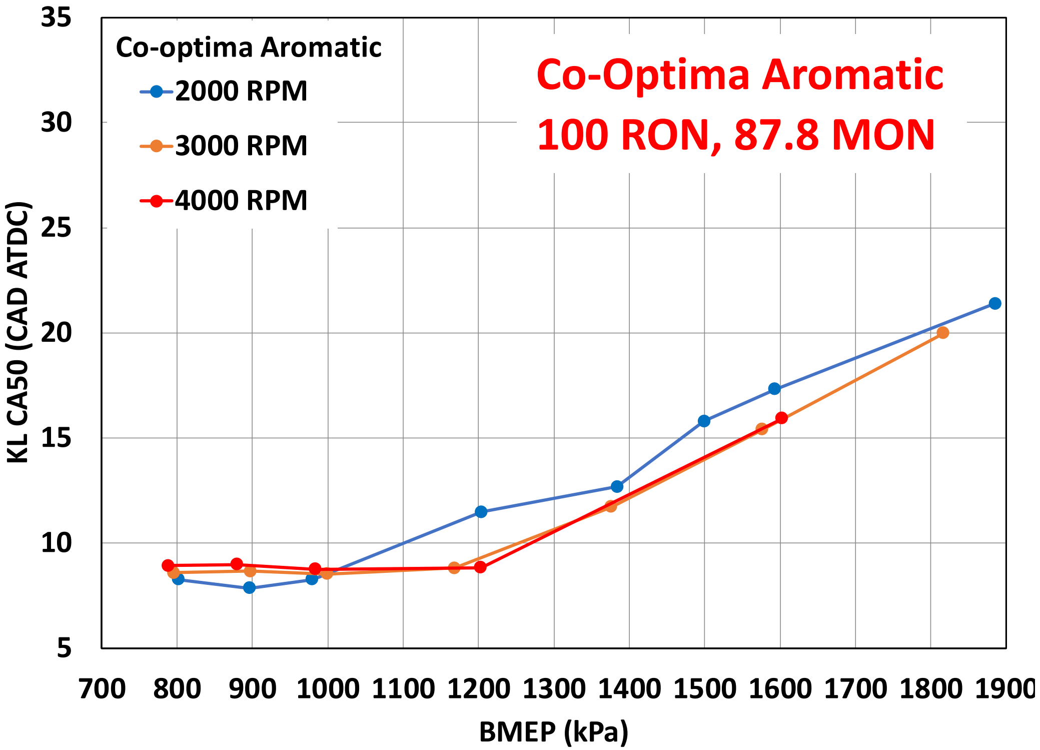
Core Fuel Co-Optima Aromatic 100 RON, 87.8 MON

- **97 RON for CR10: encounter knock at relatively high BMEP**
  - Higher CR is planned and is anticipated to magnify differences between fuels
- **Presence of LTHR causes high MON fuel to be disadvantaged at low speed**
  - MON < RON reduces combustion retard to avoid knock
- **Cross-over is a result of RON difference**
- **Observations hold for T_{Intake} = 25 and 50 °C**
  - T_{INTAKE} increased to study impact of elevated ambient Temps, reduced intercooler performance at high power conditions

For a Fixed BMEP, Combustion Phasing Advances as Engine Speed Increases but this Effect is Reduced when MON < RON

ORNL, Sluder: Accomplishments (2/3)

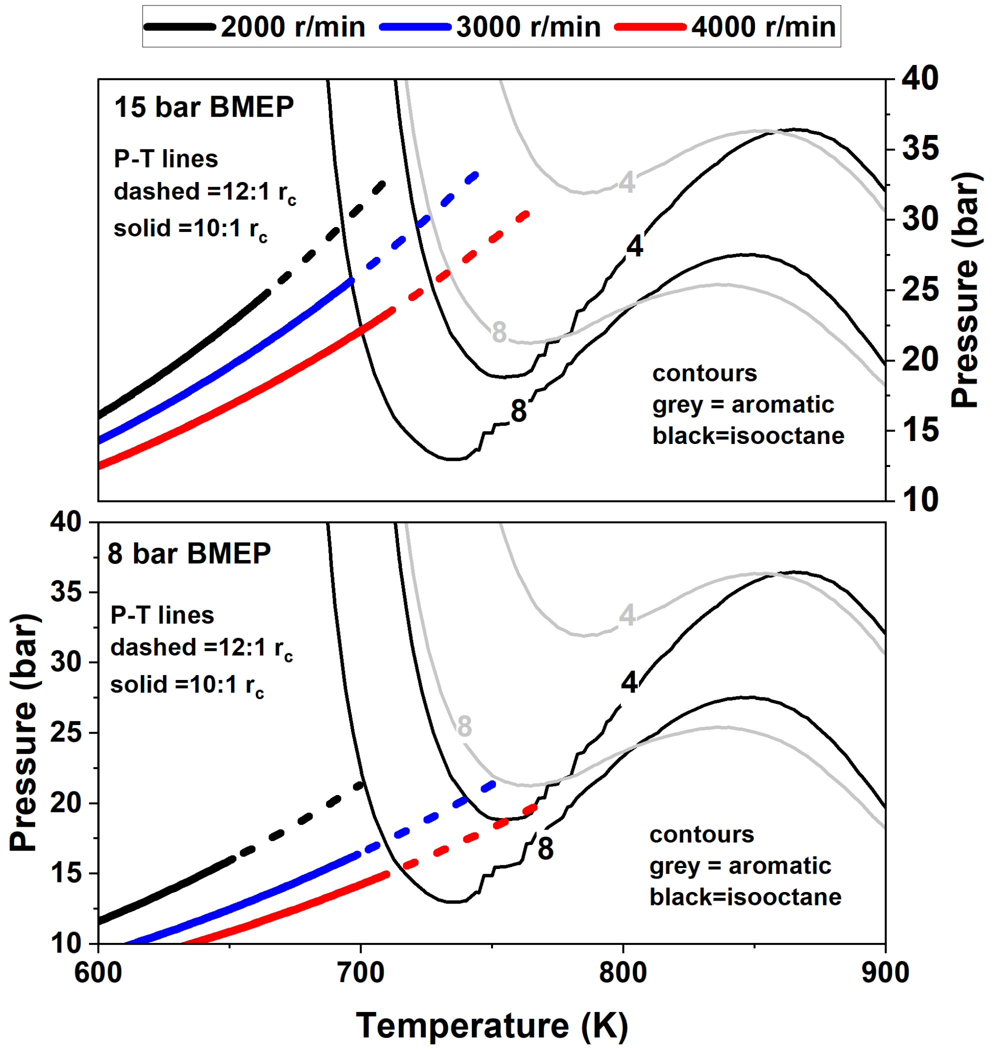




- **LTHR decreases as RPM increases: less disadvantage for high MON fuel**
- **Isooctane performance "catches up" to lower-MON aromatic fuel at high-speed, high-load conditions**
  - Elevated T_{INTAKE} conditions improve more rapidly as RPM increases
- **Data suggest isooctane performance may equal that of aromatic fuel at ~5,000 RPM**

Early Results Illustrate the Decreasing Advantage of MON < RON as Engine Speed Increases, but does not Provide Complete Understanding

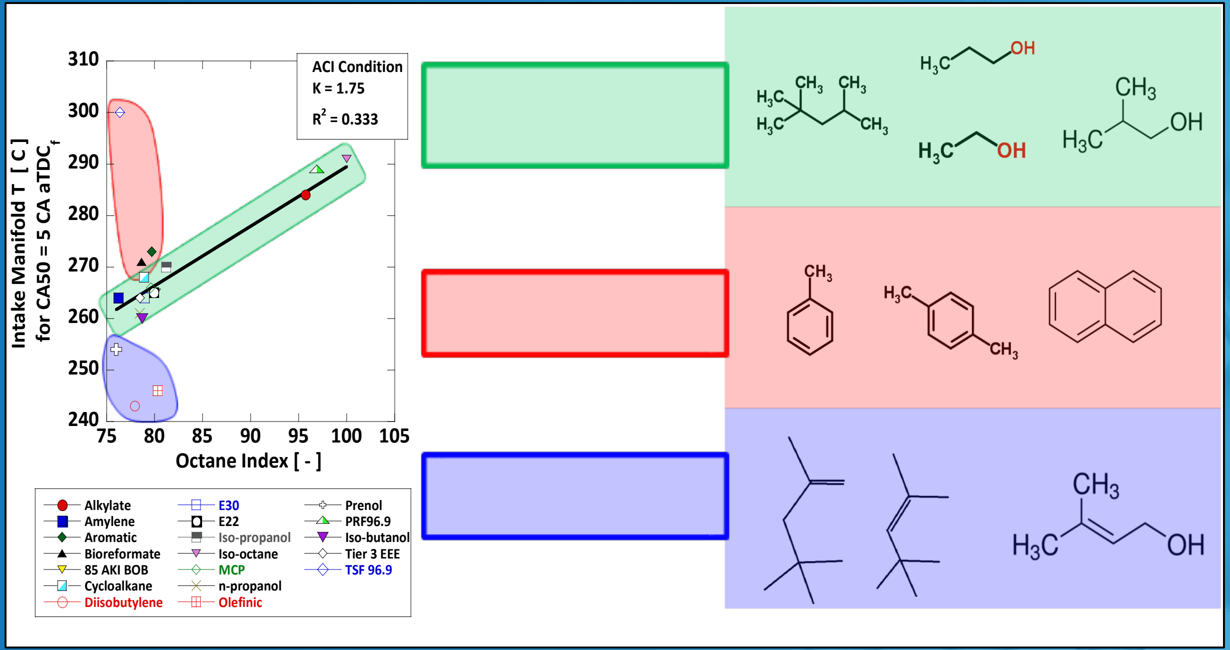
- **Do results hold as r_c increases (i.e., $r_c > 10$)?**
  - New measured r_c = 12.4 pistons installed (dashed line trajectory in PT diagram, stock 10:1 is solid lines
- **MON = RON is an extreme case.**
  - MON ~ 90 for RON = 98 produces OS = 8; more typical level
  - Add additional MON levels and fuel chemistries
- **Access P-T space differently for given T_{INTAKE}**
  - Initial results show reduced T_{INTAKE} effect with increased speed
  - Address expanded temperature studies with kinetic model
  - Fuel specific differences being explored using PT and trajectories to help elucidate observed speed and MON effects
- **What about other pairings of r_c, RON, MON?**
  - Possible to expand parametric kinetic modeling study to help provide predictive insights in high load MON and speed effects



Results Presented at 2019 AMR Suggested Fuel Properties alone were Insufficient, Fuel Chemistry Needed to be Considered

ORNL, Szybist: Approach (1/2)

Results presented at 2019 AMR for ACI Operation



- **Unlike boosted SI, OI broke down under ACI conditions**
  - Aromatics were more difficult to autoignite relative to OI expectations, requiring higher temperature intake
  - Alkanes and alcohols behaved according to OI expectations
  - Olefins were easier to autoignite relative to OI expectations, requiring lower intake temperature

Follow-on work for 2020 designed to fill-in gaps about previous conclusions

2019 ACI Condition Not Realistic for Production-Intent and/or future Multimode Engines
- Engine used standard SI valve timings, combined with very high intake temperature
- Fully homogeneous ACI was implemented, no stratification used for control
- ➢ ***Engine used for 2020 study supported by GM for multimode research, closer to production-intent configuration***

2019 Fuels Included High Concentrations on Single Components
- Diisobutylene, toluene, more, were present in high concentrations
- Not clear if conclusions were specific to these compounds, or more broadly applicable to chemical families
- ➢ ***Shell supplied set of 5 fuels blended using refinery-relevant blending streams instead of doping in individual components***

Approach: ORNL Multimode Effort used Single Cylinder Engine Supported by GM, Fuel Matrix Supported by Shell

- **GM SG2 engine provide flexible platform for multimode research**
  - Boosted SI and ACI combustion modes achieved in same engine platform without changing engine hardware (e.g., pistons, as was done in FY19 study)
- **Large matrix of 12 fuels to investigate chemistry effects**
  - 5 Co-Optima core fuels, have been used throughout Co-Optima and provide consistent point of comparison
  - 5 custom blends from Shell using refinery-relevant blending streams, do not contain high concentrations of single components
  - Representative market E10 fuel (RD5-87, used previously throughout national labs)
  - Iso-octane, for model validation
- **Three SI conditions and two ACI conditions to vary PT trajectories**
  - SI conditions investigated at intake temperatures of 35, 90, and 150 °C
  - Spark-assisted compression ignition (SACI)
  - Partial fuel stratification (PFS)

Engine Geometry of GM SG2 Installed at ORNL

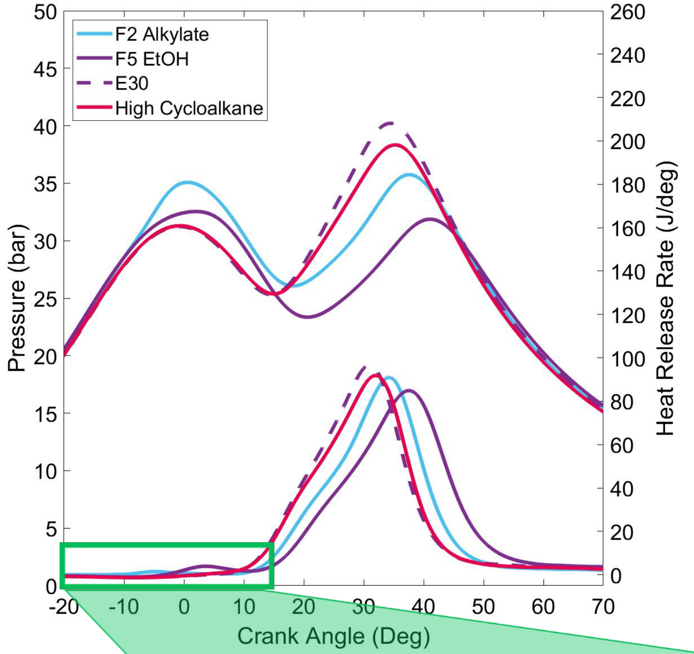
Displacement [liters]	**0.552**
Bore x Stroke [mm]	**86.0 x 94.6**
Connecting Rod [mm]	**145.5**
Compression Ratio	**12.5 : 1**
Cam Phasing	**Hydraulic phasing, 60 CAD authority for intake and exhaust**
Fuel Injector	**Central solenoid DI, 8-hole, symmetric 60° included angle**

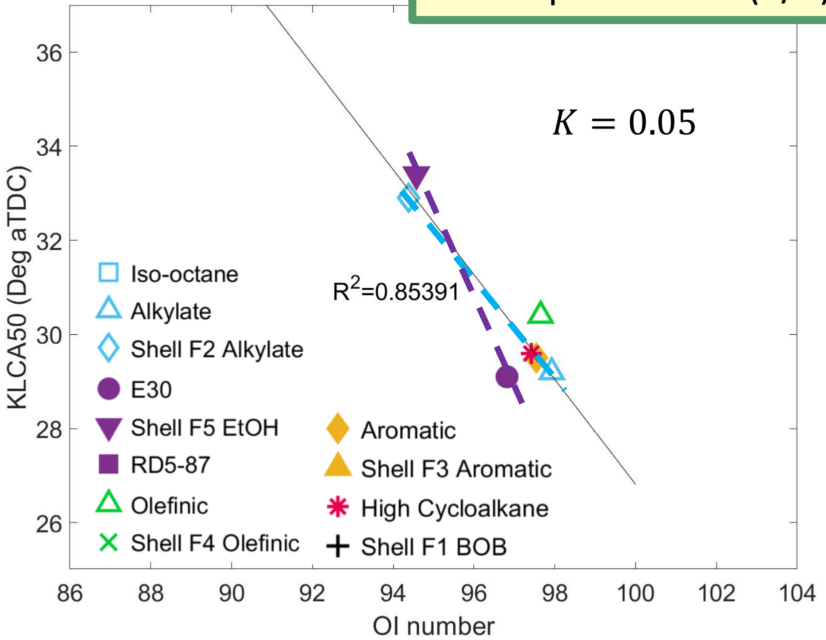
Picture of ORNL Installation of GM SG2 engine

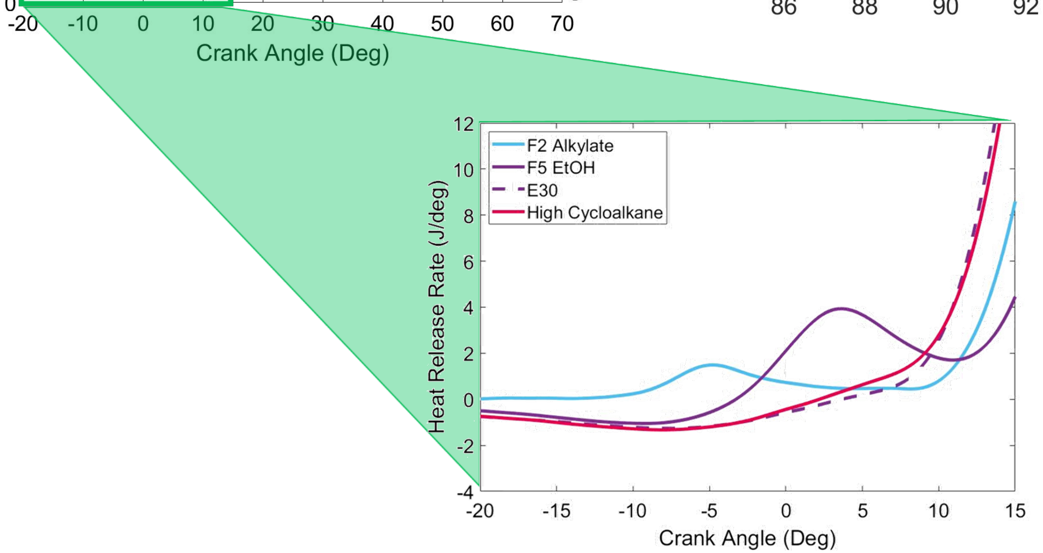
For SI Operation, OI Provides a Reasonable Correlation to Fuel Performance, Consistent with Previous Results

ORNL, Szybist: Accomplishments (1/2)

- **R^2 correlation coefficient for knock-limited phasing is 0.85**
  - Agrees well with prior ORNL results as well as literature results
- **SG2 engine enhances LTHR from mixing and compression ratio combination**
  - LTHR, or pre-spark heat release can be observed for numerous fuels
  - Fuels exhibit differences in LTHR phasing and magnitude can be useful for kinetic model validation
  - SG2 engine high CR and low charge motion allow these characteristics to be readily observed





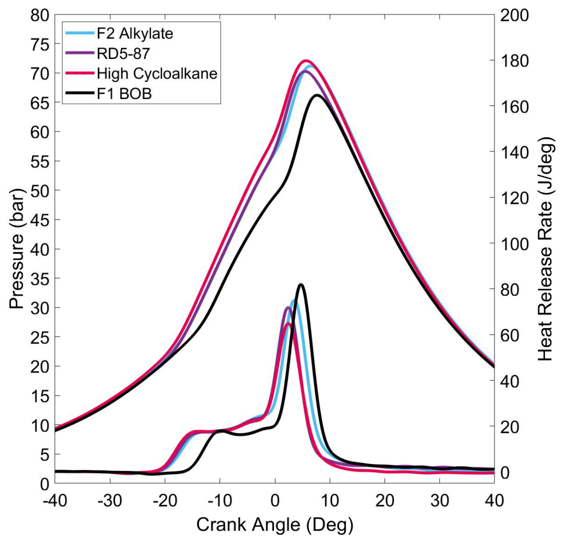


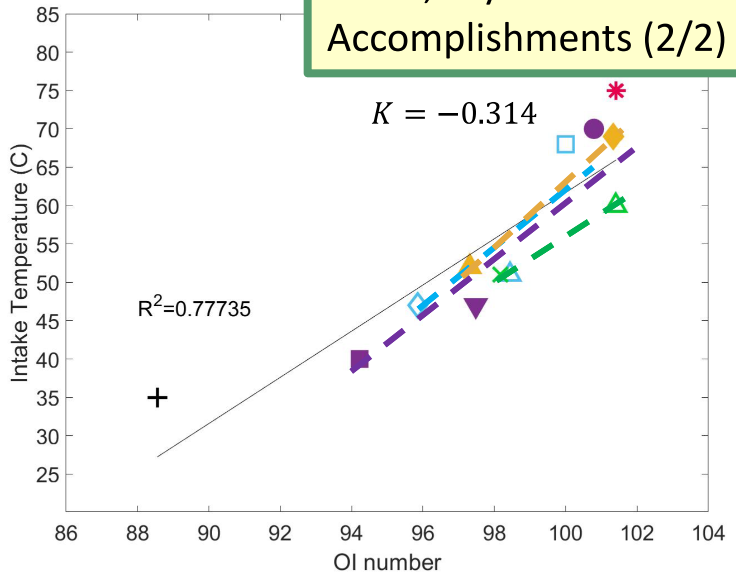
While R^2 Correlation Coefficient Remained High for ACI conditions, Fuel-Specific Trends are Observed

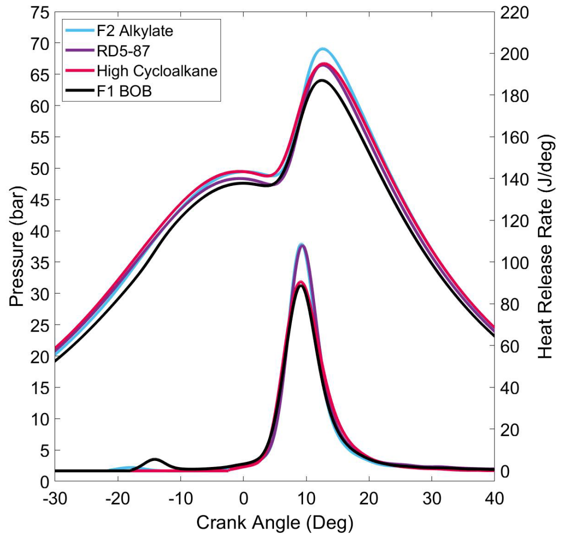
ORNL, Szybist: Accomplishments (2/2)

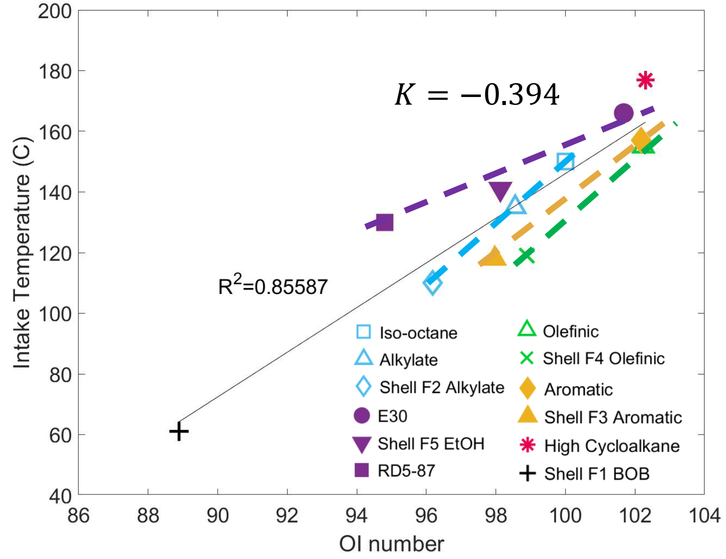
- **For ACI operating conditions, R^2 correlation coefficient for OI remained reasonably high**
- **For PFS operating condition, though, fuel-specific differences can be seen (ethanol, alkanes, aromatics, olefins)**
- **Comparing to 2019 results:**
  - Olefins remain easier to autoignite relative to OI expectations
  - Alcohols and aromatics have reversed rank ordering
- **Relative to 2019 engine conditions, these ACI conditions are more pressure-driven, produce beyond RON PT trajectories**

➢ ***Conclusion: The ACI mode that is being used will dictate correlation with OI***







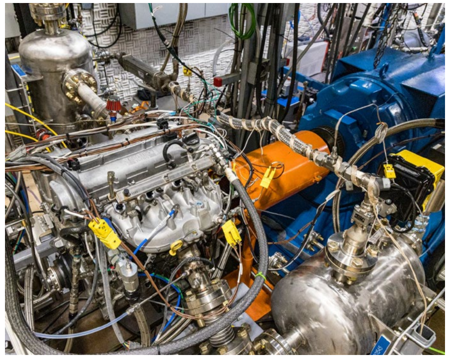


Approach: Simulations Coupling Spray and Engine Measurements Supporting Model Development and Pathways for Predictive Simulation

ANL, Som: Approach

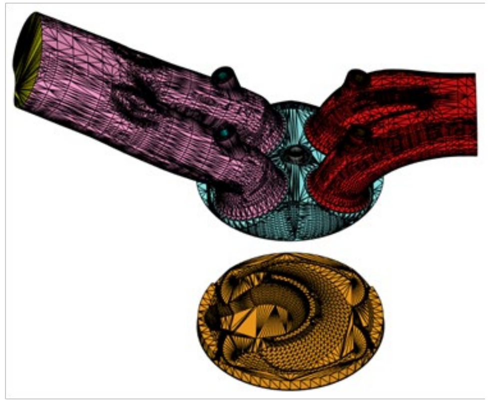
- Single-cylinder engine experiments at Oak Ridge provide baseline and engine validation data
- Constant volume vessel experiments at Sandia provide spray validation data
- Argonne leverage these data to develop CFD models able to predict SI combustion, pre-spark heat release, and investigate fuel property effects

Engine experiments



Spray validation

CFD simulations



Turbulence model:

RANS – higher throughput enabling sensitivity analysis

Spray model:

State-of-the-art Lagrangian models allowing for fuel-stratification studies

Turbulence-chemistry interaction:

Hybrid model (G-equation+ well-stirred reactor)

– improving mixed-mode prediction

Note:

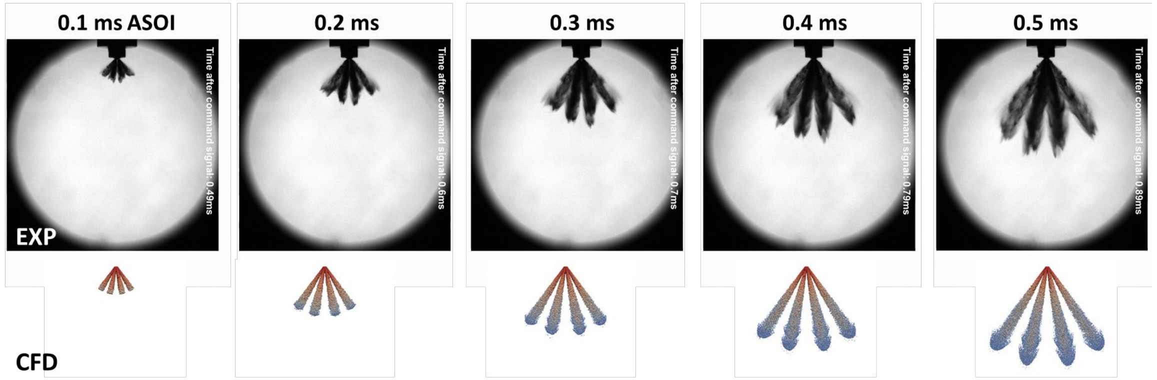
CFD work started in Oct ‘19 and experimental data of the engine were made available at the end of Feb ‘20

Simulation Predictions Well Aligned with Measured Spray Plumes and Penetration

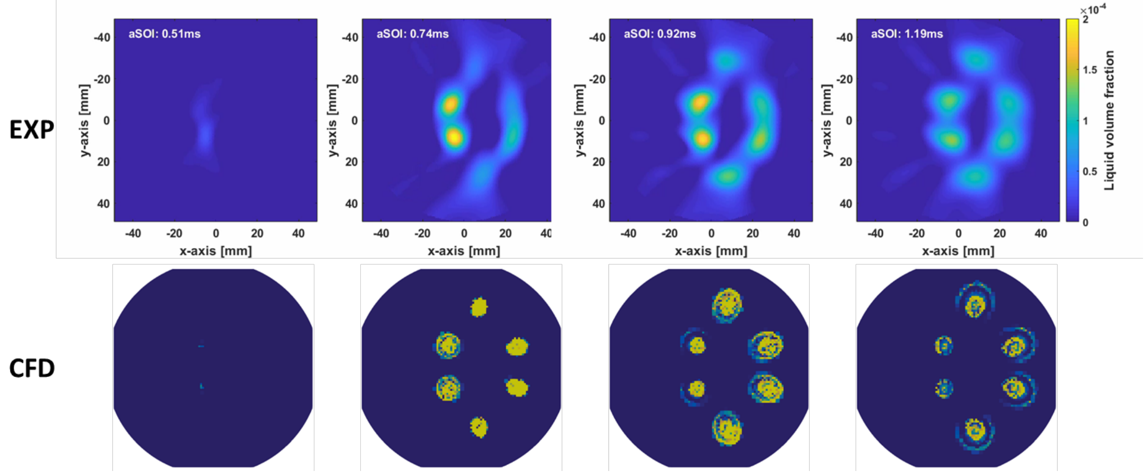
ANL, Som: Accomplishments (1/2)

Validation of Spray and Fuel Distribution

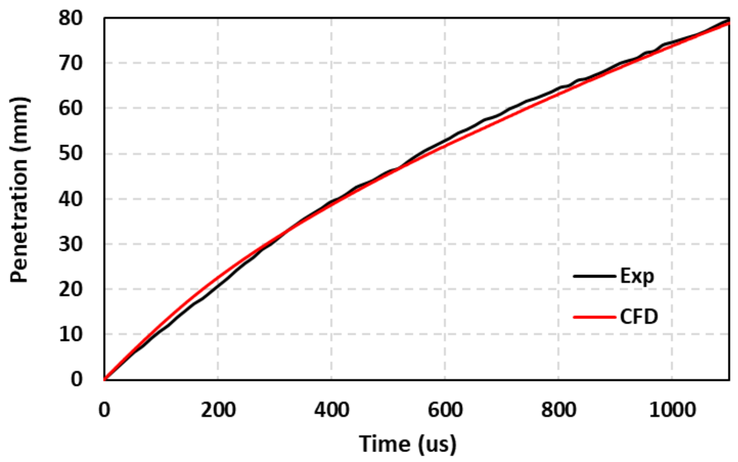
Spray morphology



Spray pattern



Spray penetration



- The spray model for the injector was validated against iso-octane experiments using high-speed extinction and laser scattering images collected at Sandia
- Calibrated spray models were able to accurately capture the spray morphology, penetration, and patterns
- **Results provided confidence for planned studies on partial fuel stratifications**

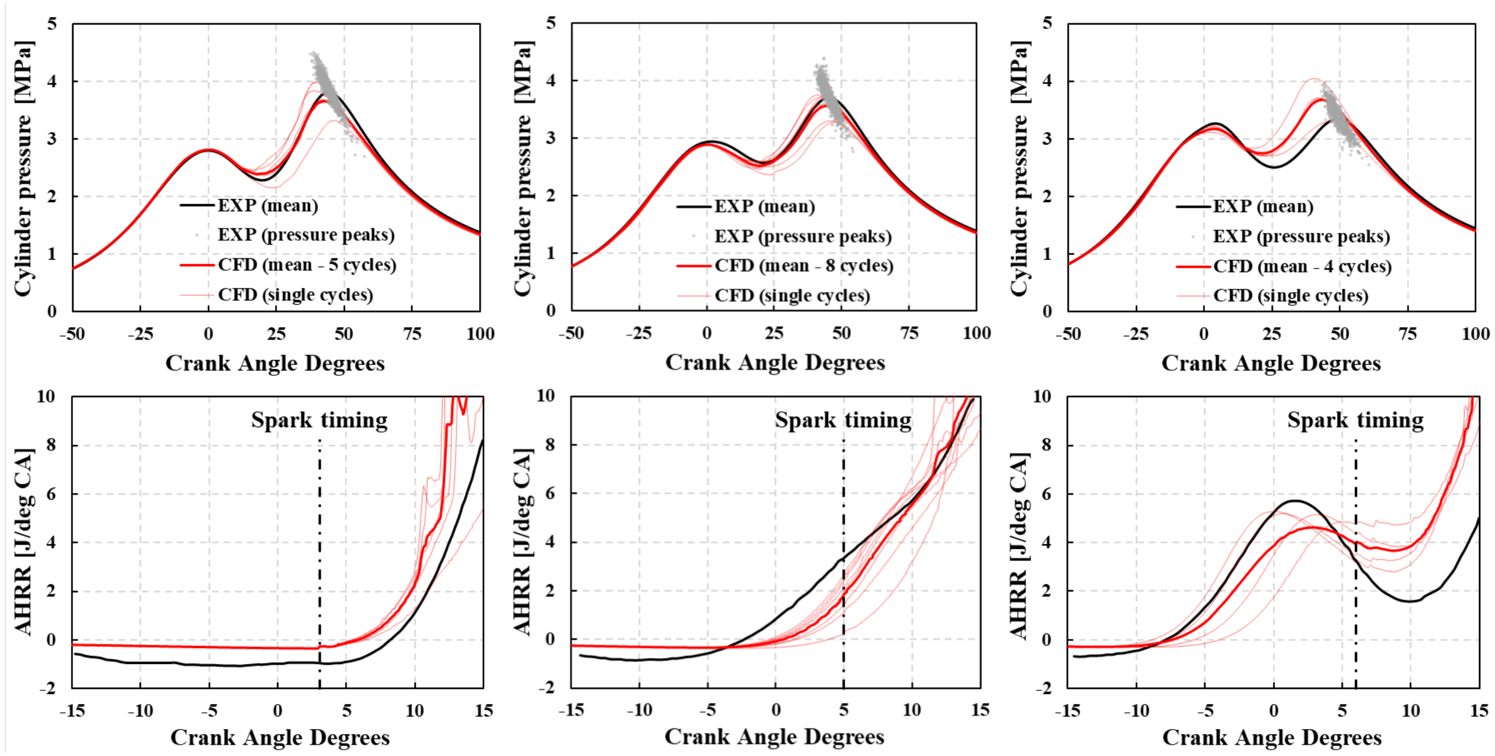
Simulation Predictions of High-Load Pre-Spark Heat Release Couple Kinetics and Fluid Mechanics to Capture LTHR and Deflagration

ANL, Som: Accomplishments (2/2)

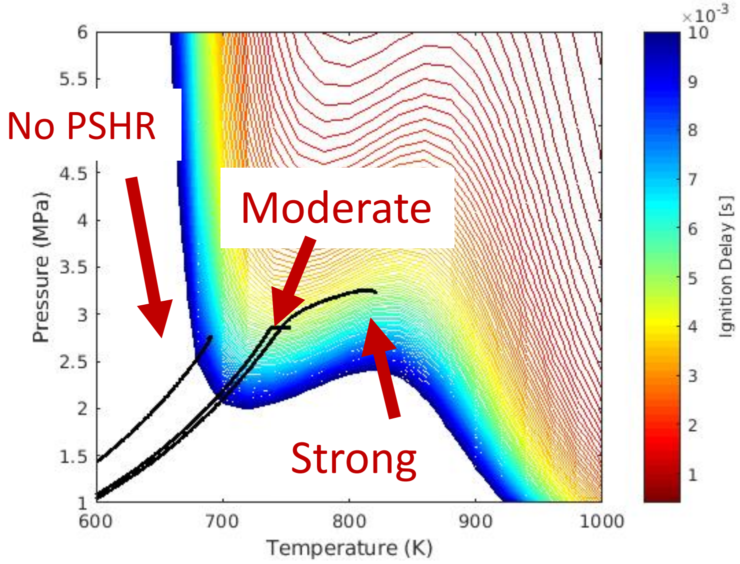
Validation on Low Temperature Heat Release (LTHR) before Spark

- Three operating conditions at 2020 rpm using Co-Optima alkylate, with different levels of pre-spark heat release (PSHR)
- **Simulations showed good predictions of PSHR and deflagration**
- On-going investigations focused on fuel effects using the P-T trajectory framework and considering phi/T stratification

No PSHR | Moderate PSHR | Strong PSHR



P-T trajectory on the ignition delay contour



Approach: ORNL High Load Effort used Single Cylinder Engine to Explore Fuel-Wall Interaction and Load on Stochastic Pre-Ignition

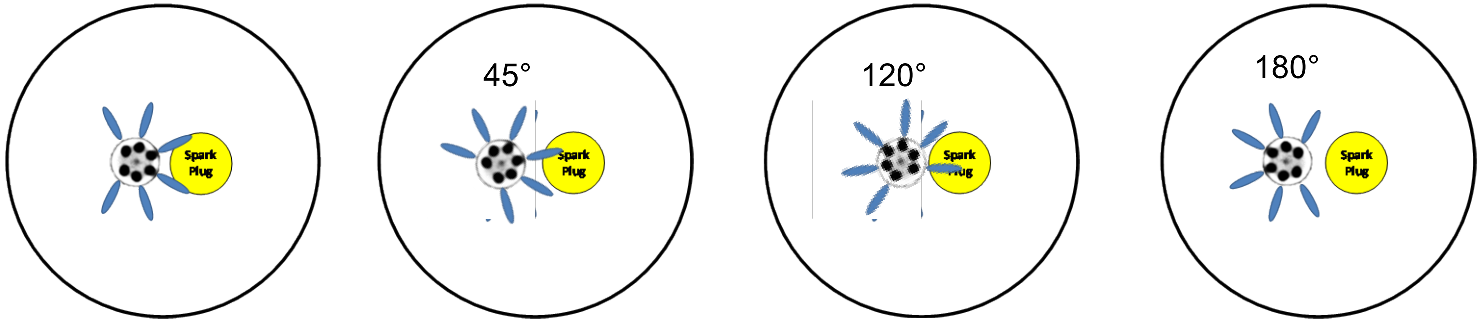
ORNL, Splitter: Approach

- **Ford 1.6L converted to single cylinder**
- **Automated test cycle repeating 10 segments of 25 minutes each**
- **Full control of all control parameters**
- **"Clock" central DI injector to match oil pressure loss (wall wetting)**
- **70 RON gasoline to match fuel kinetic state at high load**
  - Explore if fuel kinetic state, lubricant, or thermals from load are critical

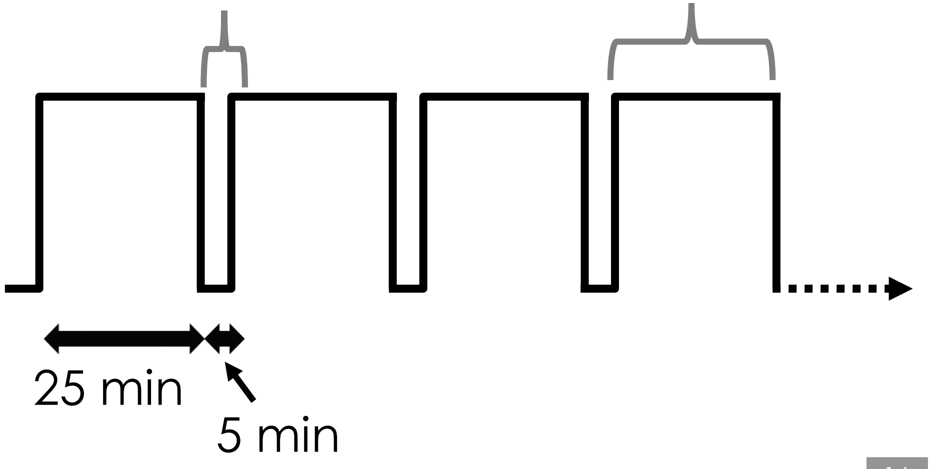
Low Load

High Load

Stock Injector Orientation | **Modified Injector Orientation** | **Modified Injector Orientation** | **Modified Injector Orientation**



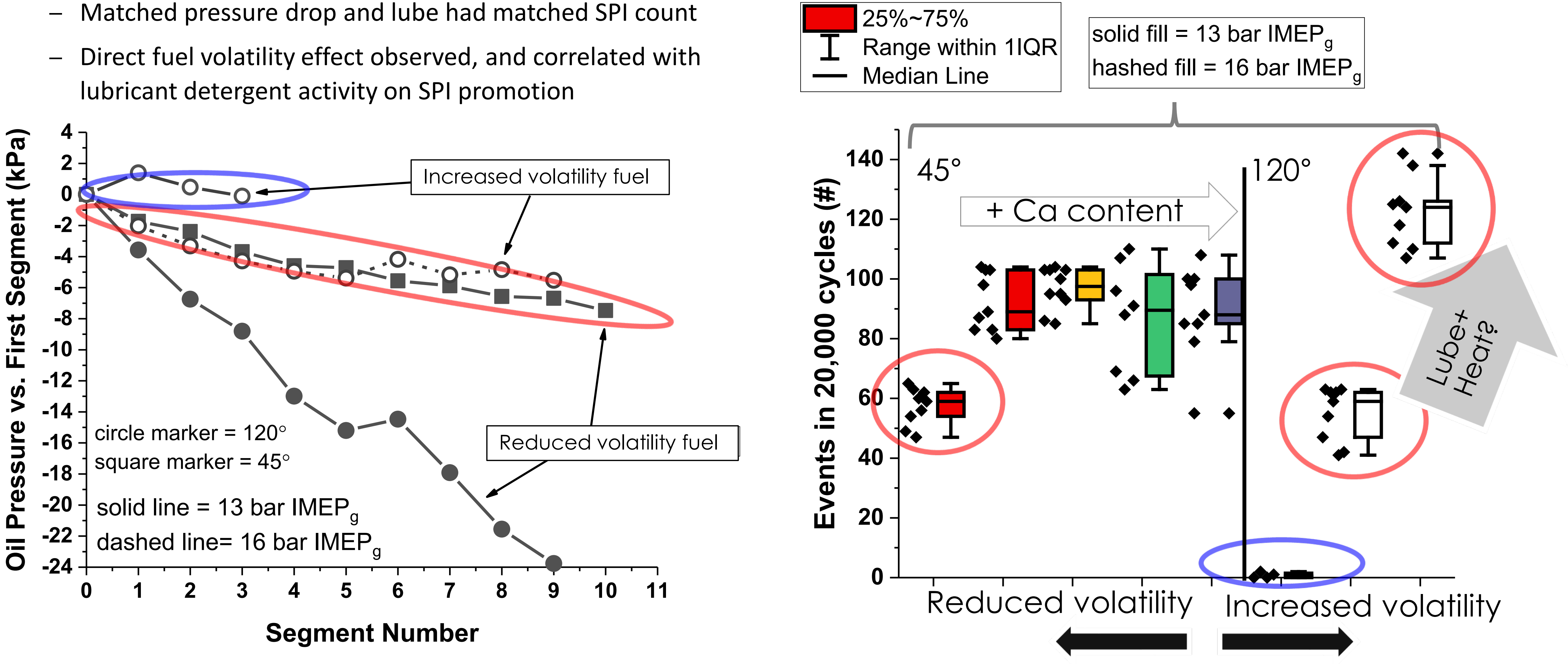
Increase fuel/wall impingement possibility



Fuel Property Effect and Engine Operating Conditions on Top Ring Zone Show Critical Activity Thresholds for Lubricant Detergent Effects on SPI

ORNL, Splitter:
Accomplishments (1/1)

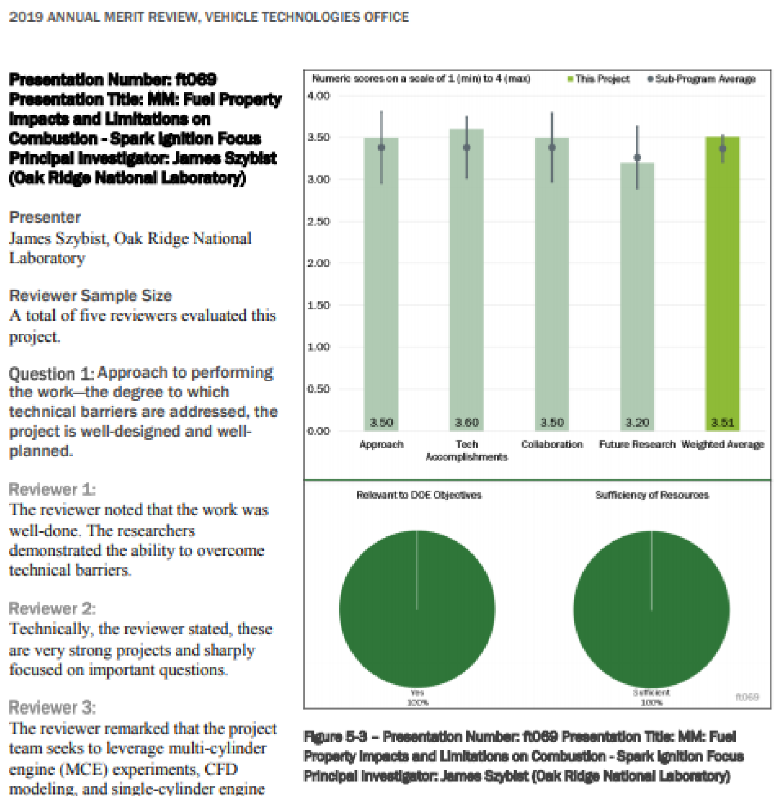
- **Oil pressure reduction from fuel dilution over time**
  - Matched pressure drop and lube had matched SPI count
  - Direct fuel volatility effect observed, and correlated with lubricant detergent activity on SPI promotion



Responses to Previous Year Reviewers' Comments
Note: Most of FY19 Work Reviewed in FT069 in 2019

- The reviewer pronounced the kinetic modeling and single-cylinder work to be outstanding and the same analysis methods have been incorporated into other workplaces.
  - **Great the hear that outputs from co-Optima are having real world impacts**
- The reviewer found the progress to be excellent but would like to have seen a greater emphasis on translating the project outcomes to simpler relationships for engine design
  - **Great feedback, we are addressing this by exploring ACI and SI with simulation and kinetic analysis tools to better understand engine design factors on multiple platforms**
- The reviewer said that the research team is using the transported Livengood-Wu integral to predict autoignition rather than advanced kinetics, presumably due to computational cost. Does the research team believe that this approach is satisfactory to simulate the OI.
  - **Yes. The L-W model uses ignition delays tabulated from detailed chemistry calculation and has similar performance in auto-ignition predictions, validated via HCCI calculations, and showed good agreement with Co-Optima merit function*.**
- The multi-cylinder work is not quite as relevant for industry; however cold and hot operation may provide other insight into the value of the different fuels.
  - **The project direction has changed and is no longer primarily focused on generating fuel consumption data. It is now focused on investigating MON effects at high loads and speeds and is investigating intake temperature and compression ratio effects**

MM: Fuel Property Impacts and Limitations on Combustion –Spark Ignition Focus,FY2019


2019 ANNUAL MERIT REVIEW, VEHICLE TECHNOLOGIES OFFICE

Presentation Number: ft069
Presentation Title: MM: Fuel Property Impacts and Limitations on Combustion - Spark Ignition Focus
Principal Investigator: James Szybist (Oak Ridge National Laboratory)

Presenter
James Szybist, Oak Ridge National Laboratory

Reviewer Sample Size
A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:
The reviewer noted that the work was well-done. The researchers demonstrated the ability to overcome technical barriers.

Reviewer 2:
Technically, the reviewer stated, these are very strong projects and sharply focused on important questions.

Reviewer 3:
The reviewer remarked that the project team seeks to leverage multi-cylinder engine (MCE) experiments, CFD modeling, and single-cylinder engine

Figure 5-3 – Presentation Number: ft069 Presentation Title: MM: Fuel Property Impacts and Limitations on Combustion - Spark Ignition Focus Principal Investigator: James Szybist (Oak Ridge National Laboratory)

*Yue and Som, Applied Energy 2019

Collaboration and Coordination with Other Institutions

Leveraging Co-Optima Collaborations:

- **Strong industry engagement including industry-led external advisory board, monthly stakeholder phone calls, and annual stakeholder meeting**
- **Collaboration across nine national laboratories, two DOE offices, and thirteen universities**
- **Co-Optima project E.1.4.2 J. Hwang & L. Pickett, providing spray data for simulation validation**

15 Industry partners in the AEC MOU

- **Meet two times a year to share information with industry partners**
- **Other national labs and University partners as well**

Direct Hardware and Fuel Support From Industry

- **Shell providing fuel with increased compositional diversity**
- **GM providing multi-mode ACI/SI relevant single cylinder hardware**
- **Ford Supporting Multi-and single cylinder engine hardware**
- **Convergent Science for support to simulation code development and resources**
- **Ansys for support to simulation resources**

Remaining Challenges and Barriers

Progress is being made, but barriers discussed in the overview slide persist.

Barriers**

USCAR Priority 1: Dilute SI Combustion

- Knock Mitigation

→ Developing a better understanding of how fuel properties can be predictive of knock

- Progress on a predictive knock model that allowed CFD-to-fuel economy estimations
- Progress showing OI is a good framework for boosted conditions
- Work remains extending this to MON-relevant pressure temperature conditions

USCAR Priority 3: Multimode ACI

- Increased tolerance to market fuel variability

→ *Developing a better understanding fuel autoignition under ACI conditions*

- Progress showing that fuel OI framework breaks down for ACI conditions, and that fuel chemistry may be important
- Work remains extending this to generalize observation
- Work remains getting to a fuel property for ACI conditions

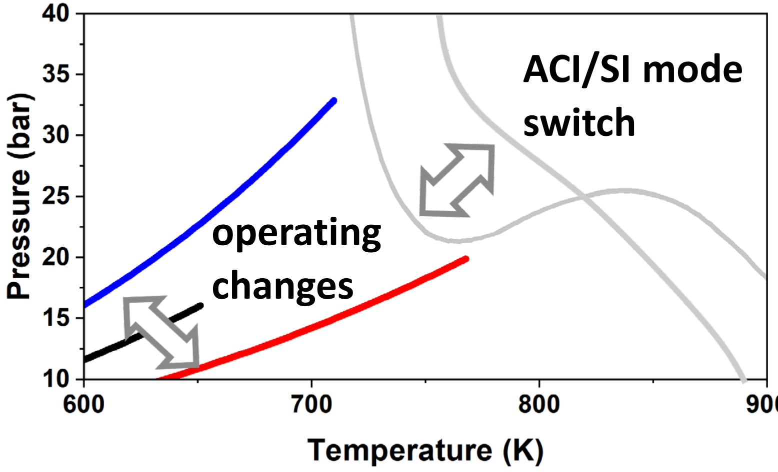
**https://www.energy.gov/sites/prod/files/2 018/03/f49/ACEC_TT_Roadmap_2018.pdf

Proposed Future Research

Any proposed future work is subject to change based on funding level

- **Identify PMI and SPI relations across a wide range of fuels**
  - Incorporate FiL diagnostic (details in ACE147) in greater capacity to study fuel effects in the top ring zone of multi mode engines
- **Developing a better understanding of the behavior of LTHR for different fuel with regards to boosted SI vs. lean ACI conditions**
- **The multi-cylinder SI work is being concluded this year, and transition work towards ACI combustion**
- **Develop a CFD capability to capture low-temperature and pre-spark heat release effects in SI/ACI multi mode engines**
- **Extension of the P-T analysis framework to consider in-cylinder thermal/phi stratification and thermodynamic property effects such as heat of vaporization and heat capacity ratio**
  - Directly applicable to multi-mode engines and defining fuel property effects on regimes, strategies, and transitions from regimes

Understanding how trajectories transition between modes and how fuel properties could be enablers



Summary

Relevance
- IC engines and the use of liquid fuels will continue to dominate transportation for many years
- Mitigation of knock is a key barrier to attaining higher efficiency for IC engines (USDRIVE roadmap)

Approach
- MCE experiments to quantify BTE improvements, feed into vehicle system, LCA, and other modeling
- Develop validated CFD models to enable investigations of isolated fuel properties in scalable manner
- SCE experiments with kinetic modeling to understand fuel properties and kinetics across PT domain

Accomplishments
- Provide foundational data and published series of octane studies with US DRIVE Fuel Working Group
- Calibrated spray models to accurately capture the spray characteristics and achieved good predictions of PSHR and deflagration
- Established kinetic framework probing PT domain with single and multi cylinder engine fuel and speed effects in multi-mode
- Discovered that engien load and fuel properties are critical for LSPI beyond fuel kinetic state alone

Collaborations
- “Co-Optima” has 9 National Labs, stakeholder engagement, and external advisory board
- Projects presented at AEC semi-annual program review, engaged with ACEC TT
- Peer-to-peer collaborations across national labs to develop modeling support for experimental efforts
- Numerous project-level collaborations direct with industry and industry consortia for support and feedback
- GM and Shell for hardware and fuel support

Future Work
- Co-Optima has identified several areas where the fuel property approach falls short of fully describing behavior in the engine. Experimental and computation investigations will be conducted to elucidate the behavior of fuel properties as they relate to OI, HoV, and LSPI.

Technical Back-Up Slides

(Include this “divider” slide if you are including back-up technical slides **[maximum of five]**. These back-up technical slides will be available for your presentation and will be included in the USB drive and Web PDF files released to the public.)

Co-Optima Aromatic Fuel Properties Compared to Alkylate and Isooctane

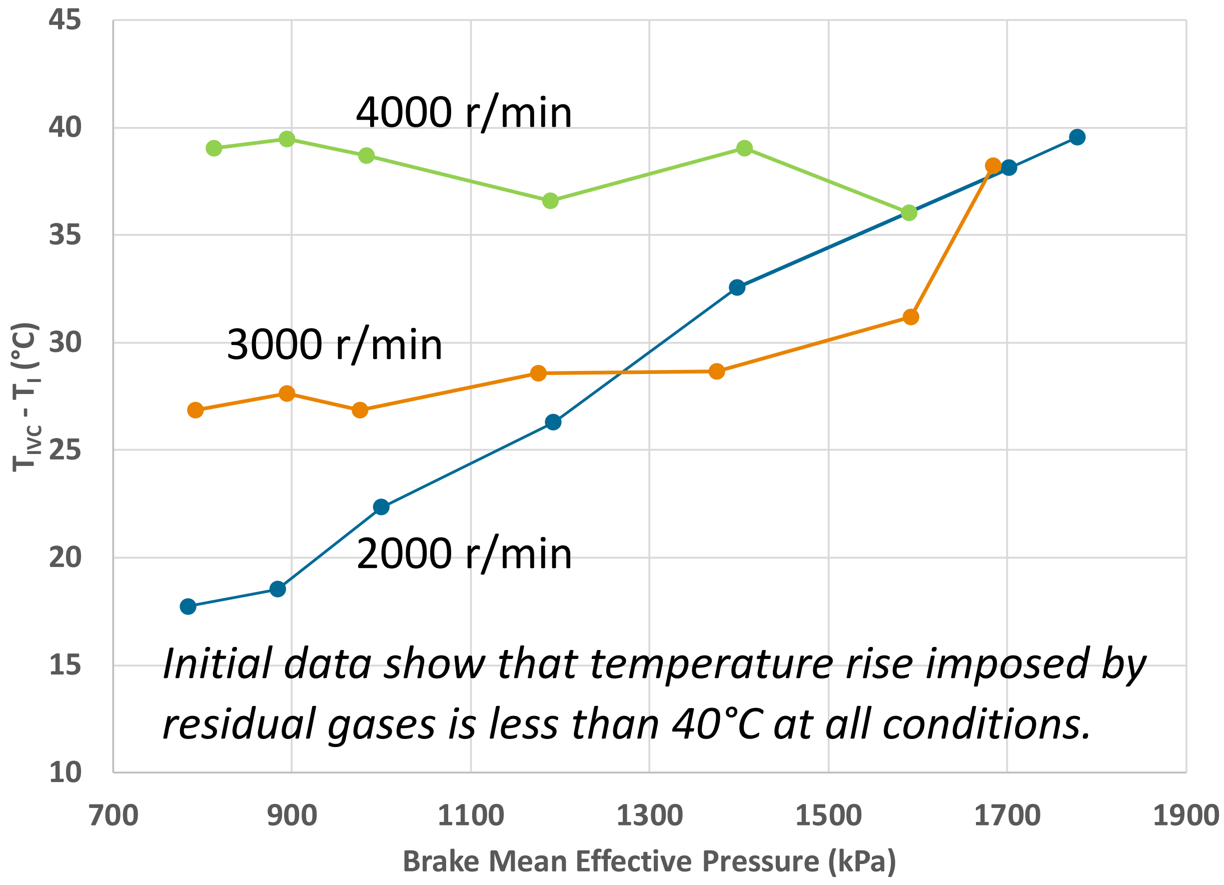
Technical Backup Slide 1

Parameter	Method	Unit	Isooctane	Co-Optima Aromatic	Co-Optima Alkylate
Research Octane Number	ASTM D2699	(-)	100	98.0	98.0
Motor Octane Number	ASTM D2700	(-)	100	96.7	96.7
Octane Sensitivity	Calculated	(-)	0	1.3	10.5
Aromatics	ASTMD1319	Vol %	-	0	35.8
Saturates	ASTMD1319	Vol %	-	100	65.0
Olefins	ASTMD1319	Vol %	-	0	4.2
Initial Boiling Point	ASTM D86	°C	-	50.3	34.3
T 10	ASTM D86	°C	-	93.1	59.4
T50	ASTM D86	°C	-	100.3	108.1
T90	ASTM D86	°C	-	105.9	157.9
Final Boiling Point	ASTM D86	°C	-	161.3	204.4
Carbon	ASTM 5291	wt %	84.21	83.75	87.22
Hydrogen	ASTM 5291	wt %	15.79	15.80	13.12
Oxygen	ASTM 5599	wt %	0	0	0
Density at 15°C	ASTM 4052	-	-	0.696	0.757
Lower Heating Value (LHV)	ASTM 4809	MJ/kg	44.300	44.520	42.950
Stoichiometric air-fuel-ratio	Calculated	-	15.15	15.17	14.52
LHV for stoichiometric mixture per kilogram of air	Calculated	MJ/kg air	2.92	2.94	2.96

Boundary Conditions Determined From Experimental Data Have Been Used to Define a Parametric Kinetic Modeling Study.

Technical Backup Slide 2

- **Boundary conditions determined from experimental measurements.**
  - Valve events measured during experiments.
  - T_{IVC} determined using Cavina model (2004) for residual gas fraction*
  - Fuel consumption vs BMEP, RPM
- **Using LLNL co-optima mechanisms.**
- **Initial Chemkin runs for experimental conditions completed for isooctane.**
- **Parametric study planned, including: CR, T_{IVC}, fuel chemistries, engine speed, fuel mass.**

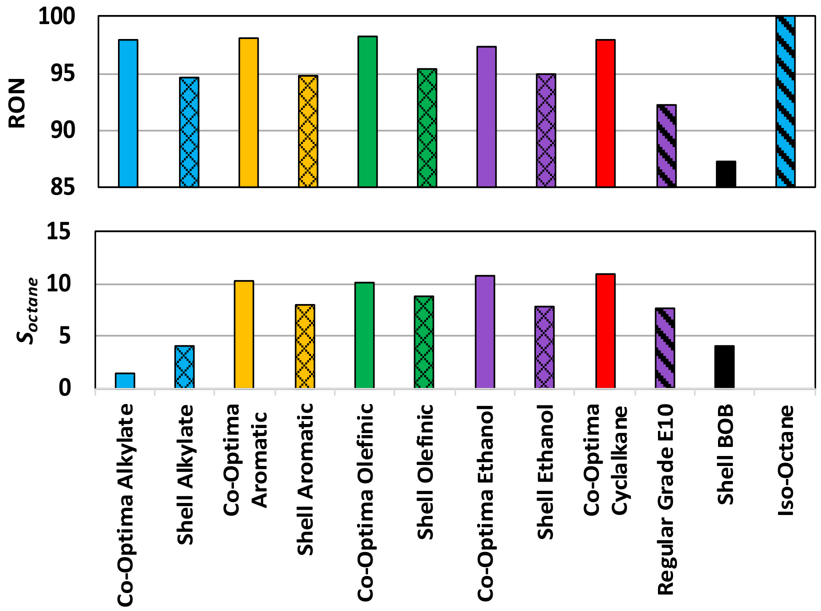


*Cavina, N., Siviero, C., and Suglia, R., "Residual Gas Fraction Estimation: Application to a GDI Engine with Variable Valve Timing and EGR," SAE Technical paper 2004—01-2943, SAE International, 2004.

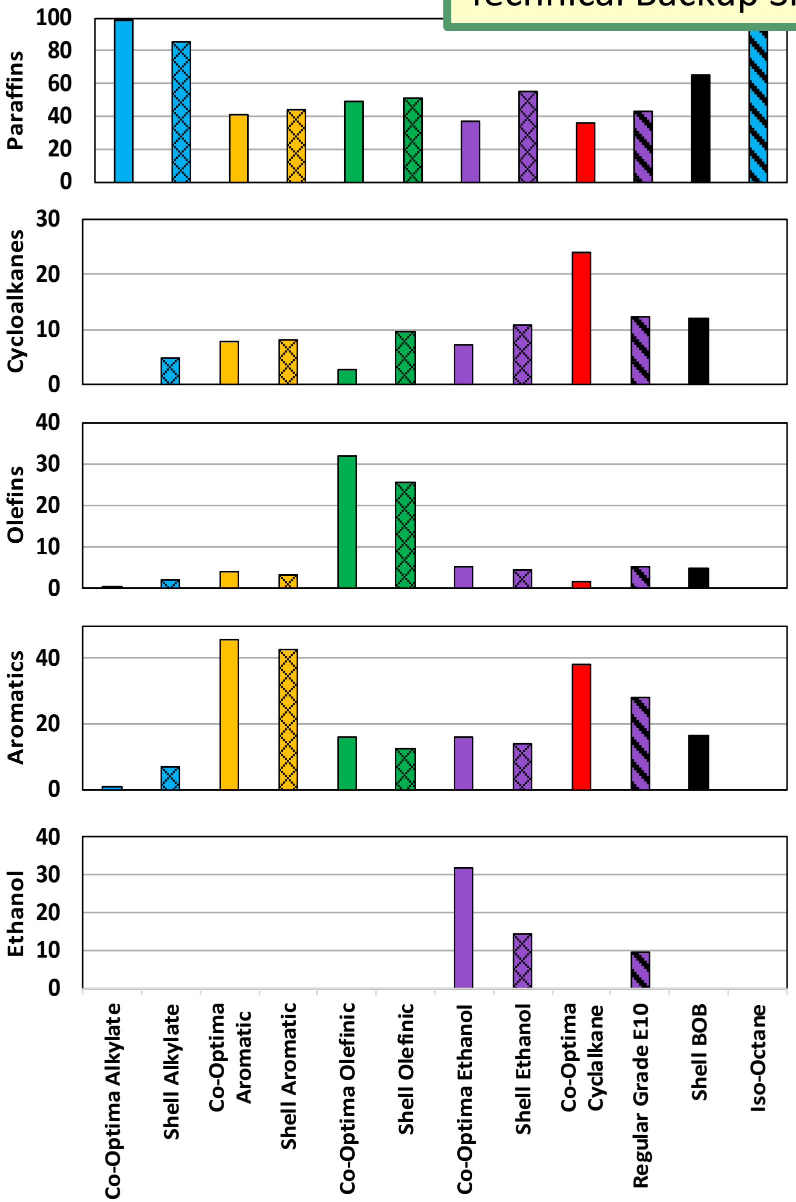
Shell Fuels and Co-Optima Core Fuels Span Similar Fuel Chemistries at Different RON and S_{octane} Target Values

Technical Backup Slide 3

- **Both fuel sets designed to investigate chemistries**
  - Paraffins
  - Aromatics
  - Olefins
  - Ethanol
- **RON Target Values**
  - Co-Optima fuels: 98.0
  - Shell fuels: 95.0
- **S_{octane} Target Values (with the exception of alkylates)**
  - Co-Optima Core Fuels: 12.0
  - Shell Fuels: 8.0



- **Shell fuels blended with refinery-relevant blending streams.**
- **Co-Optima fuel have larger single-component concentrations.**

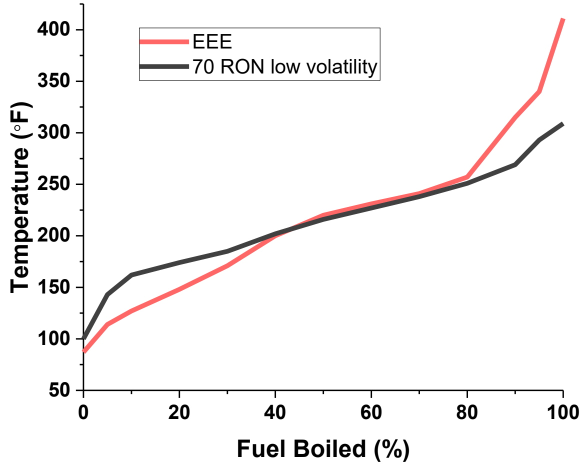


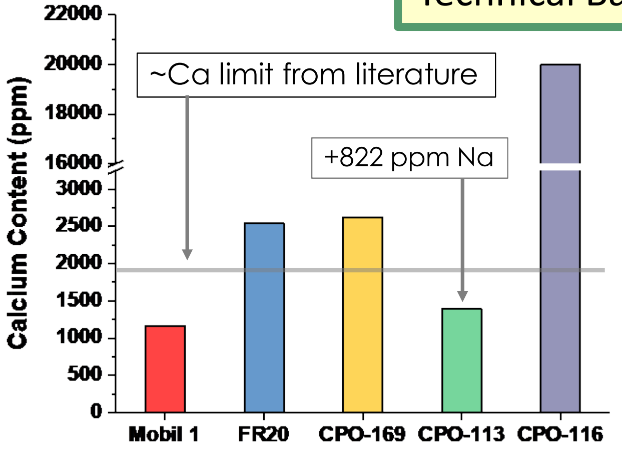
Reduced Fuel Octane Number To Explore If Similar fuel Kinetic State Could Replicate High-Load LSPI Effects at Reduced Load

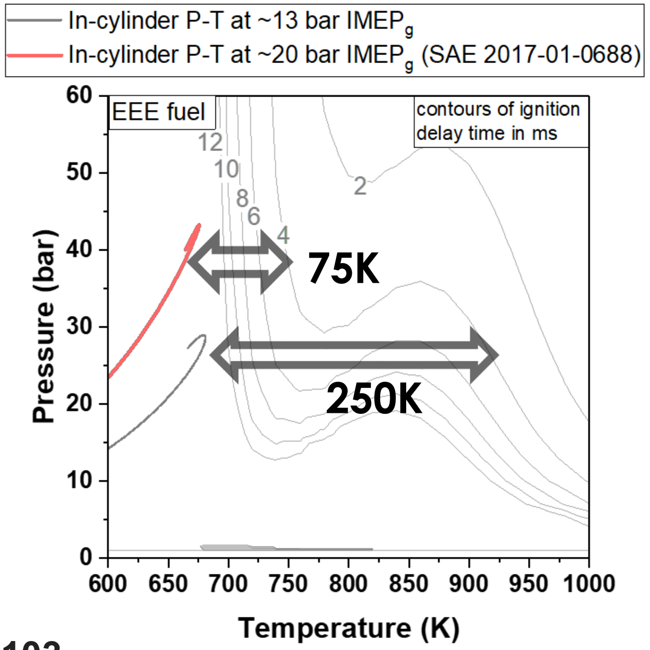
Technical Backup Slide 4

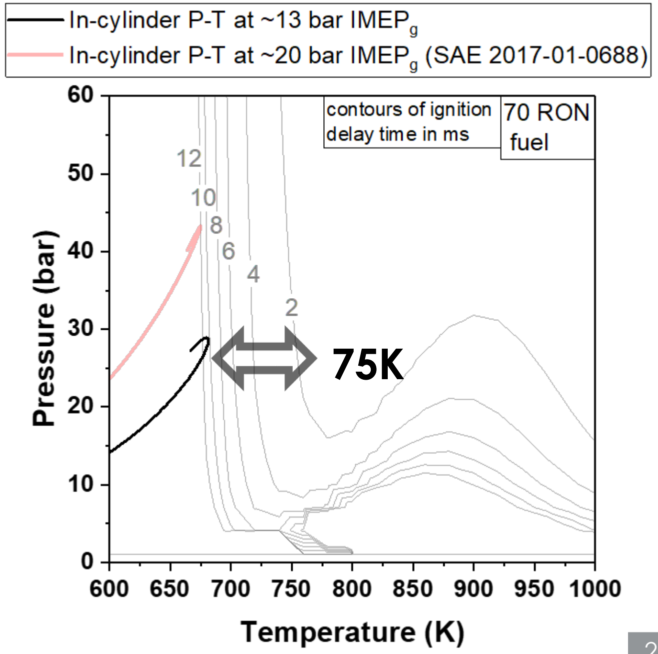
- Reduced octane number fuel with similar distillation to EEE used to move kinetic activity to reduced pressures, enabling reduced load
- Wide range of lubricant additive packages tested
- Fuel injector clocked to replicate fuel wall impingement levels at high load

	EEE	70 RON low Vol
RON (-)	96.3	71.0
MON (-)	88.8	67.7
Aromatics (%)	28.0	15.5
Olefins (%)	1.0	0.3
Saturates (%)	71.0	84.2









Splitter, D., et al., SAE 2019-24-0103